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# Ferromagnetism in epitaxial fcc Co films on Si(111)7x7 with Cu buffer layer

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**Abstract**

The magnetic properties of ultrathin epitaxial face-centered cubic (fcc) Co(111) films on Si(111)7x7 substrates with Cu buffer layer were studied experimentally and using simulation by Monte-Carlo (MC) method in frame of the ferromagnetic Ising model. For MC simulations morphology of real film acquired from images of the scanning tunnel microscopy images was used. The conditions of experimentally observed concentration phase transitions into ferromagnetic state were compared with theoretical estimations. The nature of magnetic hysteresis and temperature dependence of magnetization is discussed.



*Keywords:* cobalt; epitaxial monolayer films; STM; MOKE; Monte-Carlo method; simulation

## 1. Introduction

For many applications in modern nanoelectronics, high-spin polarization materials with good quality of interfaces are needed [1]. In this respect the epitaxial ultrathin magnetic films on semiconductor substrates represent significant interest. In these low dimensional systems grown on nonmagnetic metal substrates, the structure and magnetism of Co films are different from those of bulk Co due to reduced dimensionality. Enhanced moment and desired magnetic anisotropy could be therefore obtained in ultrathin or multilayer films in a controllable way. To explore new physics, it is usual to focus on simple

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model systems and equilibrium properties such as exchange, anisotropy, and the thermodynamic phase diagram in the space of temperature and thickness. To exploit new applications, it is typical to study more complex systems and nonequilibrium properties such as hysteresis, domain wall motion, and magnetotransport. The structure and morphology of ultrathin films are determined by phenomena occurring during growth. Therefore, it is of fundamental importance to characterize the growth process in order to achieve an efficient understanding of the relevant parameters and to be able to control the structure and morphology of the growing films to obtain the desired properties.

In previous work [2] we have been found that the coercivity of monolayers epitaxial Co(111) films deposited on epitaxial Cu(111) buffer layer on Si(111)7x7 extremely decreased with the Co coverage. For simulation we used phenomenological model of correlated states of Ising spins system. Temperature dependence of magnetization and nonequilibrium magnetic reversal process were investigated to show how real surface morphologies (extract from scanning tunneling microscopy (STM) images) can lead to observed behaviors for the coercive field of planar magnetized ultrathin films and the temperature dependence of magnetization.

## 2. Experiment

The experiments were performed in the Omicron ultra-high vacuum system. The structure of samples was Co(x)/Cu(11.5 ML)/Si(111)7x7, where x – 0.5, 1.0, 1.5, 2.0, 2.5 and 3 ML. The details of preparation and the structure of epitaxial Cu buffer layers are presented in [2]. The Co coverage is given in monolayers, where 1 ML is defined by a one-to-one atomic ratio with the Cu(111). The magnetic structure was investigated ex situ by the longitudinal magnetooptical Kerr effect (NANOMOKE-II). To prevent Co from oxidation during *ex situ* investigation, 15 ML thick Cu capping layer was formed above the Co(111) films.

## 3. Results and discussions

Fig. 1 shows the STM images of Co film at different Co coverage. At the initial stage (submonolayer Co coverage, Fig. 1a), double-atomic-layer high Co islands develop. Some of them nucleate at the flat surface and have a compact shape, the other decorate the edges of the 2D Cu islands, thus having the ring shape. At 1.5 ML of Co (Fig. 1c), the surface is still atomically rough containing three atomic levels of Co and two atomic levels of the Cu buffer (terraces and 2D islands). The 3-ML-thick Co film corresponds to the second peak in the reflection high-energy electron diffraction oscillations that have maximal amplitude. On the STM image (Fig. 1f) the surface is relatively flat as an indication of the quasi-layer-by-layer growth. However, with further Co deposition, the film again grows via 3D growth mode. It is worth to notice that conditions of Co growth on the 11.5-ML Cu buffer are similar to those reported for Co growth on the Cu(111) single crystal [3, 4], including formation of double-atomic-layer high islands and decoration of substrate steps at the initial stage and eventual growth of the pyramid-shaped epitaxial islands.

The pixels on STM-image were differentiated into some clustered cobalt atomic layers by brightness, fig. 1g. In our model, it is assumed that all underlying atomic steps are formed as solid wholly, i.e. without pores and vacancy defects in the process of the epitaxial growth. Therefore, Co-clusters were constructed by means of filling of fcc lattice in the 3D space. The part of STM-image, which corresponds to separated area on fig. 1c, is given on fig. 1g (numbers of atomic layers are the same on both images). Each pixel and, consequently, each point of model sample is, approximately, 1.443 atoms of fcc-cobalt with lattice parameter 4.089 Å. Total number of atoms N in sample of 100x100 nm 1.5 ML of Co (111) is

approximately $2.7\times10^5$. We use ranges of the pixel brightness values (0-80, 81-120, 121-150, 151-200 and 201-255) those correspond to the various heights of atomic layers.

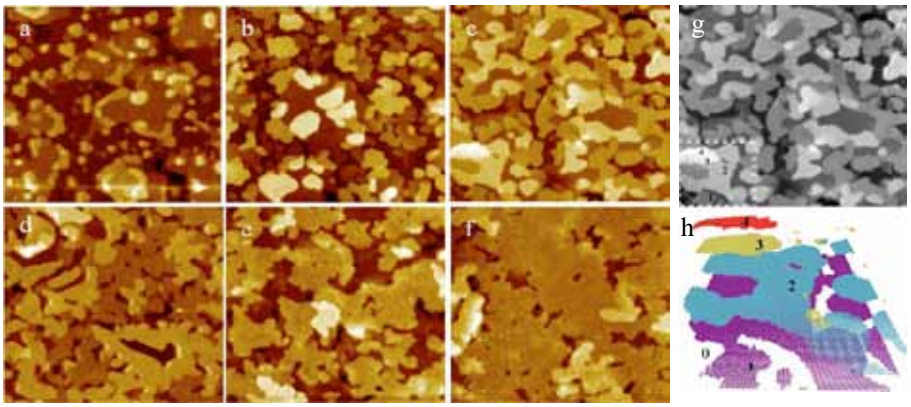


Fig. 1. STM images of epitaxial Co(111) film at Co coverage (a) 0.5 ML; (b) 1.0 ML; (c) 1.5 ML; (d) 2.0 ML; (e) 2.5 ML; (f) 3.0 ML. Image size is 100x100 nm.; (g)-(h) The model presentation of extracted field on STM Co (1.5 ML) image, (h) zoom of the STM image in the region delineated by a rectangle on (g). Four atomic layers of Co (1-4) above Cu buffer layer (0).

The simulations for fcc lattice with the highest possible number of nearest neighbors (n. n.) z = 12 were performed by the Monte-Carlo (MC) method. Each Ising spin in lattice point of simulated sample interacts with n. n. by means of the direct exchange. In simulation we have used k = 1, J = 1 in the dimensionless units. The number of MC steps for the simulations of temperature dependence of magnetization was ~10 times more than number of points in a model system.

In the proposed approach [5], the authors of the formula $p_c = 2/z$ determined the critical concentration for the appearance of ferromagnetism. The same ratio was also obtained in the percolation theory [6, 7], but for an estimation of the percolation threshold for conductive lattices with random bonds. This formula can be used here for the calculations of the critical concentration, which is needed for a phase transition into ferromagnetic state for the lattice system of spins with given number z. The theoretical estimations of $p_c$ for 1.5 ML, 2.0 ML, 2.5 ML and 3.0 ML samples are 0.55, 0.29, 0.24 and 0.21, correspondently. The mean values of the n. n. for these samples were 3.62, 6.98, 8.18 and 9.3.

Up to Co coverage of 2 ML, no longitudinal MOKE loop at RT was detected (fig. 2a). Since coverage high than 2ML MOKE measurements have revealed the ferromagnetic behavior with in-plane magnetization and practically isotropic magnetic properties. The coercive field rapidly decrease for two order of value at forming the continuous epitaxial Co film (from 2 ML to 3 ML).

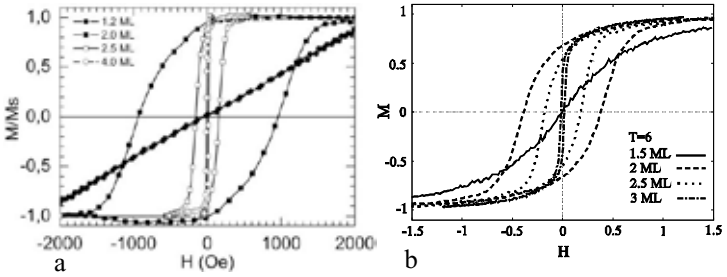


Fig. 2. Magnetic hysteresis loops for different number of monolayers. (a) – experimental, (b) – simulation at T = 6.

The automated processing of STM images in frame of the proposed computational model allows to calculate concentration as ratio between of number atoms in nanoclustered films and number of atoms in the Co layers. The simulation and theoretical estimations allow to make conclusion that the 1.5 ML sample at the low temperature is in the clustered ferromagnetic state. The simulated behaviors of the magnetizations in an external field for given samples is in agreement with theoretical estimation of critical concentration and experimental dependence of M(H). The samples with thickness 2.0 ML, 2.5 ML and 3.0 ML were in ferromagnetic state, because the condition $p > p_c$ was satisfied, in addition to the disclosing of experimental and theoretical hysteresis curves.

In the frame of the used model the magnetic hysteresis phenomenon is explained as effect of nonequlibrium in the Ising spin lattice, fig 2b. For the simulation of a nonequlibrium process in monolayered samples it was used only surface points of lattice and the number of MC steps which was proportionality quantity of a lattice cites. By this reason the system of correlated spins could not find the equlibrium configuration from the time of a field alteration, that is the cause of magnetic hysteresis in approached model.

## 4. Conclusions

We have used classical spin Ising model and morphology characteristic from STM experiments to study the magnetism of Co ultrathin epitaxial films on Si(111) by numerical simulation with Monte-Carlo method. The results of simulation and theoretical estimations are in qualitative agreement with experimental data in terms of a conditions of transition into the ferromagnetic state. We demonstrate that it is possible to qualitatively describe such important phenomenon as magnetic properties of low dimension system with simple model. For deeper insight, it necessary to take into account magnetic crystallographic anisotropy and influence of magnetostatic effects.

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